Multiscale Mathematics for Nano-Particle-Endowed Active Membranes and Films

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08/03/2016
Final Report

Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/RTA2

REPORT DOCUMENTATION PAGE

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
29-07-2016	Final Report	From 01-05-2012 to 30-04-2016

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Multiscale Mathematics for Nano-Particle-Endowed Active Membranes and Films	
	5b. GRANT NUMBER
	FA9550-12-1-0178
	5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)	5d. PROJECT NUMBER
Qi Wang (PI), M. Greg Forest (Co-PI), Peter Mucha (Co-PI), Xiaofeng Yang (Co-PI)	
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
University of South Carolina 1523 Greene St., LeConte 429 Columbia, SC 29208	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
Air Force Office of Scientific Research 875 North Randolph Street Suite 325, Room 3112 Arlington VA, 22203	AFOSR
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

DISTRIBUTION A: Distribution approved for public release.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

In this project, we conducted a systematic investigation on active liquid crystal flows and flowing polymer nano-composites including studies of nonlinear phenomenon in active magnetic mcrobead rheology, detailed analyses and simulations of active liquid crystal models in thin films, free surface geometries, and the channel geometry, applications of active liquid crystal models to complex biological systems, numerical algorithm development for multiphase fluid flows, network analysis and simulations of nanocomposite systems. We explored spatial-temporal structures using the two-scale kinetic model by mapping out the dynamics in the phase space consisting of the active parameter and the strength of active particle-particle interaction. In addition, we used a continuum active polar liquid crystal model to study the robustness of the structures and their genesis in relation to the inherent instability in the active liquid crystal model in various geometries. Network models are brought in to analyze nanocomposites transport properties and network properties of various complex networks. A series of numerical algorithms for multiphase complex fluid models are developed using a new method that we invented call energy quadratization (EQ) technique. With the new EQ technique, we designed energy stable schemes for several important model systems of multiphase viscous fluid mixtures, liquid crystal drops, active matter drops, active cells, etc, making the numerical simulation of the underlying fluids and biological objects more reliable.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
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AFOSR Final Report

PI: Qi Wang, University of South Carolina
Co-PIs: Xiaofeng Yang, University of South Carolina
&
M. Greg Forest and Peter Mucha, University of North Carolina at Chapel Hill

In this project, we conducted a systematic investigation on active liquid crystal flows and flowing polymer nano-composites including studies of nonlinear phenomenon in active magnetic mcrobead rheology, detailed analyses and simulations of active liquid crystal models in thin films, free surface geometries, and the channel geometry, applications of active liquid crystal models to complex biological systems, numerical algorithm development for multiphase fluid flows, network analysis and simulations of nanocomposite systems. In the study of active liquid crystals, we explored spatial-temporal structures using the two-scale kinetic model by mapping out the dynamics in the phase space consisting of the active parameter and the strength of active particle-particle interaction. In the meantime, we used a reduced order, continuum active polar liquid crystal model to study the robustness of the structures and their genesis in relation to the inherent instability in the active liquid crystal model. Detailed studies are conducted with respect to channel flows and free surface filament flows which have direct relevance to various engineering and biological applications. Network models are brought in to analyze nanocomposites transport properties and network properties of various complex networks.

New numerical algorithms are developed for a host of multiphase phase field based hydrodynamic models, in which a new method called Energy Quadratization or EQ was invented to systematically linearize transport equations derived from the generalized Onsager principle. These new methods are then applied to efficiently integrate the governing system of equation for the active matter systems are continuously improved.

We present experimental data and numerical modeling of a nonlinear phenomenon in active magnetic microbead rheology that appears to be common to entangled polymer solutions (EPS). Dynamic experiments in a modest range of magnetic forces show (1) a short-lived high viscosity plateau, followed by (2) a bead acceleration phase with a sharp drop in apparent viscosity, and (3) a terminal steady state that we show resides on the shear-thinning slope of the steady-state flow curve from cone and plate data. This latter feature implies a new protocol to access the nonlinear steady state flow curve for biological EPS available only in microliter-scale volumes. We use the moment closure form of the Rolie–Poly kinetic model for EPS hydrodynamics, together with a decoupling approximation that obviates the need for a full three-dimensional (3D) flow solver, to qualitatively reproduce this dynamic experimental sequence. We thereby explain the phenomenon in terms of entangled polymer physics, and show how the nonlinear event

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(acceleration and termination on the shear-thinning response curve) is tunable by the interplay between molecular-scale mechanisms (relaxation via reptation and chain retraction) and magnetic force controls. The experimental conditions mimic movement of cilia tips, bacteria, and sperm in mucus barriers, implying a physiological relevance of the phenomenon and compelling further quantitative kinetic-flow 3D numerical modeling.

We have developed a set of kinetic models and simulation tools to study anisotropic nano-particle dispersions and active particle dispersions to generate spatial-temporal structures that the ensemble can exhibit. Using the kinetic models, we have investigated the spatial-temporal structure of the model solutions. In the end, we have obtained the phase diagram for the solutions in the important model parameters. Using a coarse-grain model for active polar liquid crystals, we analytically and numerically explored the spatial-temporal patterns in active particle systems and studied the solution instability in details in channel flows and free surface liquid filaments. In particularly, we investigated the capillary instability of a falling active liquid crystal filament and discovered a stunning set of instabilities due to the activities of the liquid crystal molecules or active nanoparticles. We anticipate that this will lead to new applications of active particle dispersions in material processing and interpretation for capillary dynamics in biological systems.

After quenching/annealing, we adopt the statistics in the probability density function to analyze the materials properties, primarily electric properties, using network models and assessment tools developed for community networks. The work performed builds on kinetic models and corresponding solution algorithms for processing conditions of nano-particle-endowed films, coatings and membranes. Drawing from databases generated by these codes, we are actively investigating network-mediated properties that are not well-modeled by homogenization theory. We have explored DC resistive electrical response of connected nanorod composites at particle volume fractions above the percolation threshold. These calculations are performed in the high aspect ratio conductivity limit, wherein only currents along particulates are considered. As an extension of the above investigation, and as a means towards understanding the general behaviors observed there, we have also considered similar effects and observations obtained in the classic "random resistor" setting of bond percolation on 3D cubic lattices. We have also investigated dielectric properties at particle volume fractions below the percolation threshold. In these calculations, the associated network is an all-to-all capacitance network.

New and efficient numerical algorithms for multiphase fluid flows formulated using phase field are developed to decouple the momentum transport equation from the phase transport equations making the numerical computational tool more robust and modular. Some of these numerical schemes are applied to study cellular aggregate fusions and liquid jet dynamics of liquid crystal polymers.

We also applied the active liquid crystal models and the numerical technology to develop a set of new models and simulation tools for cell motion in mitosis and migration on patterned substrate. These models are being used in collaboration with applied physicists

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and material scientists to study the interaction between the cell and the substrate material in order to design novel cell-sensing and guiding materials.

5 PhD students have been partially supported by this award during their graduate studies. They have graduated and move on to either continue their postdoc training or working in universities and industries.

The team has been very productive during the last four years. Papers published and submitted in the period are listed below:

Publications:

1. Chen Chen and Qi Wang, "3-D Pattern Formation in Biofilms," Contemporary Mathematics (586), 2013, 105-116.
2. Yi Sun and Qi Wang, "Modeling and Simulations of Multicellular Aggregate Self-assembly in Biofabrication Using Kinetic Monte Carlo Methods," Soft Matter, 2013, 9, 2172-2186.
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37. Jia Zhao, Xiaofeng Yang, Jun Li and Qi Wang, "Energy stable numerical schemes for a hydrodynamic model of nematic liquid crystals." Siam J. Sci. Comp., in press, 2016.

38. Ya Shen, Jia Zhao, César de la Fuente-Núñez, Zhejun Wang, Robert E. W. Hancock, Clive R. Roberts, Jingzhi Ma, Jun Li, Markus Haapasalo and Qi Wang, "Development and Experimental Validation of a Model for Oral Multispecies Biofilm Recovery after Chlorhexidine Treatment", Scientific Reports, 6, 2016, 27537.

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43. Jia Zhao, Tianyu Zhang, and Qi Wang, "Treatment of Biofilms by Nanotechnology and Applications to Food Science," NANOTECHNOLOGY IN FOOD SCIENCESE, editor, Van de Voorde Marcel, Springer-Verlag, Berlin, 2016.

PhD graduates of Qi Wang, Forest and Mucha supported in part by this contract:

1. Jia Zhao, University of South Carolina, 2012-2016, PhD May 2015, University of South Carolina, June 2015-Juky 2016, University of North Carolina at Chapel

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Hill, July 2016-present
2. Norazaliza Mond Gamil, PhD May 2015, Universiti Malaysia Pahang, 2015-present
3. Chen Chen, PhD August 2012, Citibank, 2013-present
4. Feng (Bill) Shi, PhD May 2013, University of Chicago, Computation Institute, June 2013 - present
5. Simi Wang, PhD May 2014, Amazon, May 2014 - present

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Multiscale Mathematics for Nano-Particle-Endowed Active Membranes and Films

Grant/Contract Number
AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".

FA9550-12-1-0178

Principal Investigator Name
The full name of the principal investigator on the grant or contract.

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Abstract

In this project, we conducted a systematic investigation on active liquid crystal flows and flowing polymer nano-composites including studies of nonlinear phenomenon in active magnetic mcrobead rheology, detailed analyses and simulations of active liquid crystal models in thin films, free surface geometries, and the channel geometry, applications of active liquid crystal models to complex biological systems, numerical algorithm development for multiphase fluid flows, network analysis and simulations of nanocomposite systems. We explored spatial-temporal structures using the two-scale kinetic model by mapping out the dynamics in the phase space consisting of the active parameter and the strength of active particle-particle interaction. In addition, we used a continuum active polar liquid crystal model to study the robustness of the structures and their genesis in relation to the inherent instability in the active liquid crystal model in various geometries. Network models are brought in to analyze nanocomposites transport properties and network properties of various complex networks. A series of numerical algorithms for multiphase complex fluid models are developed using a new method that we invented call energy quadratization (EQ) technique. With the new EQ technique, we designed energy stable schemes for several important model systems of multiphase viscous fluid mixtures, liquid crystal drops, active matter drops, active cells, etc, making the

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2. New discoveries, inventions, or patent disclosures:

Do you have any discoveries, inventions, or patent disclosures to report for this period?

No

Please describe and include any notable dates

Do you plan to pursue a claim for personal or organizational intellectual property?

Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

Extensions granted or milestones slipped, if any:

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

2. Thank You

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